# PHASE DIAGRAM OF THE SPIN-1 ANISOTROPIC HEISENBERG MODEL WITH A SINGLE-ION ANISOTROPY

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**ABSTRACT.** The spin-1 anisotropic Heisenberg model with a single-ion anisotropy is studied using the Oguchi's pair approximation. Although the theory is developed for lattices with general coordination number, we treat in detail the three-dimensional lattice with the lowest coordination number, i.e. diamond lattice, where the critical and tricritical behavior of the system is analyzed as a function of both the single-ion anisotropy and exchange anisotropy.

## INTRODUCTION

The investigation of critical behavior of quantum Heisenberg systems, which are useful for the description of many magnetic materials, belongs among the most plentiful areas of statistical physics. In recent years, the special attention has been devoted to the low dimensional spin-1 Heisenberg models [1-4]. Pan and Wang analyzed the effect of a single-ion anisotropy on the ground-state properties of the spin-1 Heisenberg model for a general lattice [5]. However, as far as we know, similar treatment of thermodynamic properties at non-zero temperatures has not been done up to now. Therefore, the purpose of this paper is to study the criticality and tricriticality of the spin-1 anisotropic Heisenberg model with a single-ion anisotropy for lattices with general coordination number.

## MODEL AND ITS SOLUTION

The Hamiltonian of the spin-1 Heisenberg system in a presence of the single-ion anisotropy $D$ and the external magnetic field $h$ is described as

$$\begin{aligned} H &= -\sum_{(i,j)} J[\Delta(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z] \\ &\quad -D\sum_i (S_i^z)^2 - h\sum_i S_i^z, \end{aligned} \qquad (1)$$

where the first term represents the anisotropic exchange interaction. $J$ is the exchange coupling constant ($J > 0$) restricted to the nearest-neighbour pairs of spins and $\Delta$ is the exchange anisotropy parameter ($\Delta$=0 and $\Delta$=1 correspond to the Ising and isotropic Heisenberg models, respectively). Finally, $S_i^\gamma$ ($\gamma = x, y, z$) are the components of the spin-1 operator at sites $i$.

Since the inplementation of single-ion anisotropy $D$ in the system under investigation can potentially lead to first-order phase transitions, we need to know the expression of free energy in order to distinguish the stable and unstable magnetic phases. Due to this fact we adopt the simple Oguchi's pair approximation (OA) [6], which is superior to the mean-field method. Thus, the Hamiltonian (1) in the OA for a cluster with two spins is given by

$$\begin{aligned} H_{ij}^{OA} &= -J[\Delta(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z] \\ &\quad -D[(S_i^z)^2 + (S_j^z)^2] - h_{ef}(S_i^z + S_j^z), \end{aligned} \qquad (2)$$

in which $h_{ef}$ is the effective field, acting on both the spins of cluster, of the form $h_{ef} = J(q-1)m + h$. $q$ is the coordination number of the lattice and $m$ is the magnetization per site, i.e. $m = \langle \frac{1}{2}(S_i^z + S_j^z)\rangle$.

The Hamiltonian $H_{ij}^{OA}$ in the matrix representation calculated within a standard basis set of functions $|S_i^z, S_j^z\rangle$ ($S_i^z = \pm 1, 0$ and $S_j^z = \pm 1, 0$) can be written in the form of $9 \times 9$ matrix. Then it is quite straightforward to obtain nine eigenvalues by diagonalizing the matrix of $H_{ij}^{OA}$. Thus, the partition function $Z = \mathrm{Tr}_{ij}\exp(-\beta H_{ij}^{OA})$ has the following form

$$\begin{aligned} Z &= e^{\beta(-J+2D)} + 2e^{\beta(J+2D)}\cosh(2\beta h_{ef}) \\ &\quad +2e^{\beta(D-J/2)}\cosh[\beta\sqrt{(D-J/2)^2 + 2J^2\Delta^2}] \\ &\quad +4e^{\beta D}\cosh(\beta J\Delta)\cosh(\beta h_{ef}), \end{aligned} \qquad (3)$$

where $\beta = 1/k_B T$ is the reciprocal temperature ($k_B$ is the Boltzmann constant). The knowledge of the partition function allows us to express the relations for all thermodymanic quantities. The free energy of the two-spin cluster is then defined as

$$f = -\beta^{-1}\ln Z + J(q-1)m^2, \qquad (4)$$

wheares the magnetization $m$ per site is obtained by minimizing the free energy (4) and is given by

$$\begin{aligned} m &= \frac{1}{Z}\{2e^{\beta(J+2D)}\sinh(2\beta h_{ef}) \\ &\quad +2e^{\beta D}\cosh(\beta J\Delta)\sinh(\beta h_{ef})\}. \end{aligned} \qquad (5)$$

Through the use of Eqs. (4) and (5) we can completely analyze the phase diagrams of the present model.

Indeed, close to the second-order phase transition from the ordered phase ($m \neq 0$) to the paramagnetic one ($m = 0$) the magnetization $m$ is very small, for $h = 0$, and one may expand Eq. (5) into the form

$$m = am + bm^3 + cm^5 + ..., \qquad (6)$$

where the coefficients $a, b$, and $c$ are functions of $T, J, D, \Delta$, and $q$. So, hereby the second-order transition line occurs when $a = 1$, $b < 0$ and the tricritical

point is determined by conditions $a = 1$, $b = 0$, and $c < 0$. On the other hand, the first-order phase transitions between different phases can be obtain from a comparison of their free energies.

## RESULTS AND DISCUSSION

Now, let us study the phase diagram of the system and the thermal variations of magnetization for the case of diamond lattice ($q = 4$) in zero external magnetic field. The choice of this lattice is motivated by the fact that the diamond lattice is a three-dimensional lattice with the lowest coordination number and hence, one should expect the most obvious impact of quantum fluctuations on the cooperative ordering.

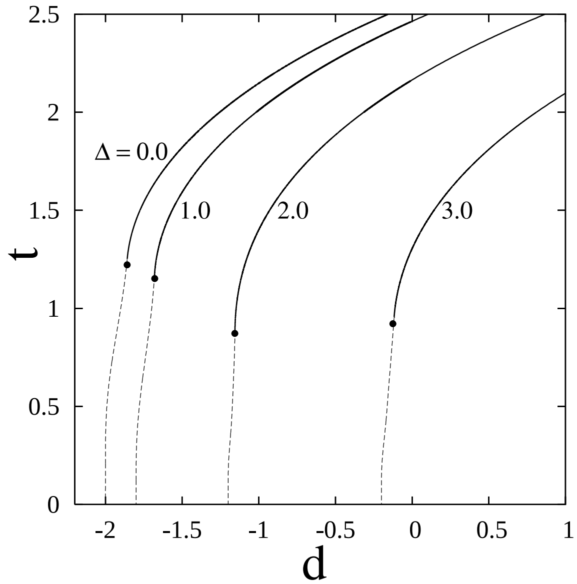


Fig. 1. The phase diagram of the spin-1 anisotropic Heisenberg model.

The phase diagram in the reduced units $d = D/J$ and $t = k_B T/J$ for different values of $\Delta$ is shown in Fig. 1. The solid and dashed lines represent the second- and first-order phase transitions, respectively. The black circles denote the positions of tricritical points ($TCP$). As one can see from this figure, the temperature of second-order phase transitions gradually declines with decrease of $d$, for any value of $\Delta$, until the $TCP$ is reached, where the phase transitions change from the second-order to first-order ones. By further decreasing of $d$ the correspondent first-order phase transition lines fall smoothly to zero. It is noteworthy that the temperature of second-order phase transitions, in the limit $d \to \infty$, does not depend on the anisotropy parameter $\Delta$ and is equal to $t^{\star} = 4.5392$. Hereafter, it is evident from Fig. 1 that the present system exhibits the highest critical temperatures in the Ising limit ($\Delta = 0$). On the other hand, the exchange anisotropy strengthening gradually decreases the critical temperature as a result of raising quantum fluctuations. Finally, an increase of the anisotropy parameter $\Delta$ causes a shift of $d$-coordinate of tricritical point ($d_t$) to the higher values. To illustrate the effect of single-ion anisotropy on the phase transitions we show in Fig. 2 the thermal variations of magnetization $m$ in the case of isotropic model ($\Delta = 1$) for some appropriate values of $d$. It is obvious from the figure that for $d = -1.65$ and $-1.68$ the magnetization falls smoothly to zero when temperature approaches the critical temperature $t_c$. This behavior of magnetization is typical for the continuous phase transitions and persists until $d > d_t$ ($d_t = -1.6801$ for $\Delta = 1$). On the other

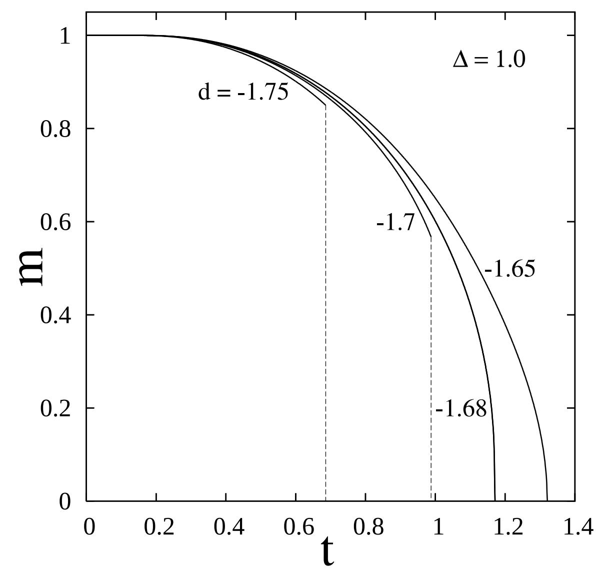


Fig. 2. The temperature behavior of magnetization of the spin-1 isotropic Heisenberg model for several values of $d$. The dashed lines typify the discontinuity of magnetization at the temperature of first-order phase transition.

hand, further reducing of parameter $d$ induces the occurence of discontinuity in the magnetization at the critical temperature $t_c$ what is characteristic for the first-order phase transitions. It is noteworthy that this discontinuity increases when the single-ion anisotropy $d$ further retreats from the value $d_t$.

## CONCLUSIONS

In this paper, the phase diagram of the spin-1 anisotropic Heisenberg model with the uniaxial single-ion anisotropy is examined within the framework of the Oguchi's pair approximation. We have demonstrated that both the exchange anisotropy $\Delta$ as well as single-ion anisotropy $d$ have a significant influence on the criticality and tricriticality of the model under investigation. Finally, it should be mentioned that the more comprehensive results of our investigation will be published in the near future.

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